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The effect of microstructure on lattice thermal conductivity of ScN thin films

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Thermoelectric applications require materials with low lattice thermal conductivity. Thus the knowledge of lattice thermal conductivity of materials under realistic conditions is vitally important. Here we have studied the effect of microstructure on lattice thermal conductivity of ScN thin films using a theoretical model based on a new *ab initio* description that includes the temperature dependence of the interatomic force constants, and treats anharmonic lattice vibrations [1-3]. We compare the results with the experimental data by Time Domain Thermoreflectance (TDTR). ScN is selected as a model system because its power factor is large (2.5×10^{-3} $Wm^{-1}K^{-2}$ at 800K) while the thermal conductivity is high, yielding low thermoelectric figure of merit (ZT) of about 0.2 [4]. Thus, reduction of the lattice thermal conductivity is needed. Our results show a trend of reduction in lattice thermal conductivity with decreasing grain size, with good agreement between the theoretical model and experimental data. Therefore we suggest a possibility to control thermal conductivity by tailoring the microstructure of ScN. More importantly, we provide a mathematical tool to predict the effect of the microstructure on the lattice thermal conductivity of materials based on first-principles calculations.

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